

Extended proof of Annex B.2 of Neural Ordinary differential equation

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Let

1. $f(z(t), \theta(t), t) = \frac{dz(t)}{dt}$

2. $Z = [z(t), \theta(t), t]$

3. $a(t) = \frac{dL}{dZ(t)} = \left[\frac{dL}{dz(t)}, \frac{dL}{d\theta(t)}, \frac{dL}{dt} \right] = [a_z(t), a_\theta(t), a_t(t)]$

4. $g(Z(t), t) = \frac{dZ(t)}{dt} = \left[\frac{dz(t)}{dt}, \frac{d\theta(t)}{dt}, \frac{dt}{dt} \right] = [f, \mathbf{0}_{\mathbf{E}}, 1]$ where $\mathbf{0}_{\mathbf{E}}$ is a null matrix of appropriate size

Then, we can define

$$Z(t + \varepsilon) = Z(t) + \int_t^{t+\varepsilon} g(Z(t), t) dt = T_\varepsilon(Z(t), t)$$

notice that

$$a(t) = \frac{dL}{dZ(t)} = \frac{dL}{dZ(t+\varepsilon)} \frac{dZ(t+\varepsilon)}{dZ(t)} = a(t+\varepsilon) \frac{\partial T_\varepsilon(Z(t), t)}{\partial Z(t)}$$

Thus we can derive $a(t)$:

$$\begin{aligned}
\frac{da(t)}{dt} &= \lim_{\varepsilon \rightarrow 0^+} \frac{a(t+\varepsilon) - a(t)}{\varepsilon} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{a(t+\varepsilon) - a(t+\varepsilon) \frac{\partial}{\partial Z(t)} T_\varepsilon(Z(t), t)}{\varepsilon} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{a(t+\varepsilon) - a(t+\varepsilon) \frac{\partial}{\partial Z(t)} (Z(t) + \varepsilon g(Z(t), t) + \mathcal{O}(\varepsilon^2))}{\varepsilon} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{a(t+\varepsilon) - a(t+\varepsilon) \left(I + \varepsilon \frac{\partial g(Z(t), t)}{\partial Z(t)} + \mathcal{O}(\varepsilon^2) \right)}{\varepsilon} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{-\varepsilon a(t+\varepsilon) \frac{\partial g(Z(t), t)}{\partial Z(t)} + \mathcal{O}(\varepsilon^2)}{\varepsilon} \\
&= \lim_{\varepsilon \rightarrow 0^+} -a(t+\varepsilon) \frac{\partial g(Z(t), t)}{\partial Z(t)} + \mathcal{O}(\varepsilon) \\
&= -a(t) \frac{\partial g(Z(t), t)}{\partial Z(t)}
\end{aligned}$$

As you can see, the proof of appendix B.1 holds for any vector Z . What's more interesting is the way we can exploit this to get $\frac{da_\theta(t)}{dt}$:

$$-a(t) \frac{\partial g(Z(t), t)}{\partial Z(t)} = [a_z(t), a_\theta(t), a_t(t)] \cdot \begin{pmatrix} \frac{df(z(t), \theta(t), t)}{dz} & \frac{df(z(t), \theta(t), t)}{d\theta} & \frac{df(z(t), \theta(t), t)}{dt} \\ \frac{d\theta/dt}{dz} & \frac{d\theta/dt}{d\theta} & \frac{d\theta/dt}{dt} \\ \frac{dt/dt}{dz} & \frac{dt/dt}{d\theta} & \frac{dt/dt}{dt} \end{pmatrix}$$

But as mentioned in the paper, $\frac{d\theta(t)}{dt} = 0$ and $\frac{dt}{dt} = 1$ which means that the second and third rows are null (derivatives of constants). Hence:

$$\begin{aligned}
-a(t) \frac{\partial g(Z(t), t)}{\partial Z(t)} &= [a_z(t), a_\theta(t), a_t(t)] \cdot \begin{pmatrix} \frac{df}{dz} & \frac{df}{d\theta} & \frac{df}{dt} \\ \mathbf{0_E} & \mathbf{0_E} & \mathbf{0_E} \\ \mathbf{0_E} & \mathbf{0_E} & \mathbf{0_E} \end{pmatrix} = \\
&= - \begin{bmatrix} a_z(t) \frac{df}{dz} + a_\theta \mathbf{0_E} + a_t \mathbf{0_E} \\ a_z(t) \frac{df}{d\theta} + a_\theta \mathbf{0_E} + a_t \mathbf{0_E} \\ a_z(t) \frac{df}{dt} + a_\theta \mathbf{0_E} + a_t \mathbf{0_E} \end{bmatrix} = - \begin{bmatrix} a_z(t) \frac{df}{dz} \\ a_z(t) \frac{df}{d\theta} \\ a_z(t) \frac{df}{dt} \end{bmatrix}
\end{aligned}$$

Now, we've got:

$$\frac{da(t)}{dt} = - \left[a_z(t) \frac{df}{dz}, a_z(t) \frac{df}{d\theta}, a_z(t) \frac{df}{dt} \right] = - \frac{d}{dt} \left[\frac{dL}{dz(t)}, \frac{dL}{d\theta(t)}, \frac{dL}{dt} \right]$$

Hence:

$$\begin{aligned} \frac{d}{dt} \left(\frac{dL}{d\theta(t)} \right) &= -a_z(t) \frac{df}{d\theta} \\ \implies \frac{dL}{d\theta(t)} &= - \int a_z(t) \frac{df}{d\theta} dt \end{aligned}$$